wwPDB EM Validation Summary Report

Oct 27, 2024 – 11:30 PM EDT

PDB ID	:	8E5A
EMDB ID	:	EMD-27908
Title	:	Human L-type voltage-gated calcium channel Cav1.3 treated with 1.4 mM Sofosbuvir at 3.3 Angstrom resolution
Authors	:	Gao, S.; Yao, X.; Yan, N.
Deposited on	:	2022-08-20
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

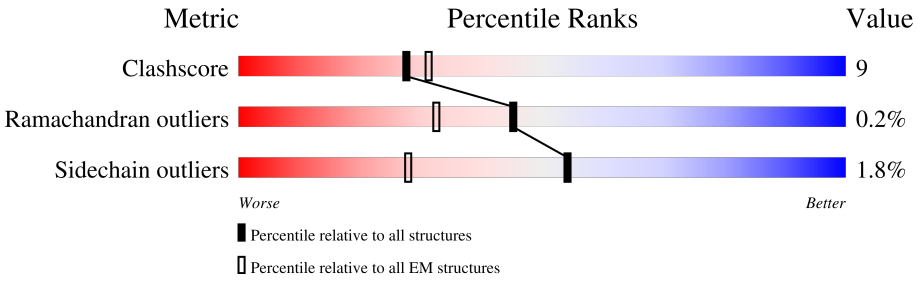
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2161	16% 44% 12% · 43%
2	D	1103	11% 70% 15% 14%
3	C	484	67% 49% 18% 33%
4	B	3	67% 33% 33% 33%
5	E	2	100% 100%
5	G	2	50% 100%
5	H	2	50% 50% 50%
6	F	4	50% 50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1230	9900	6517	1597	1715	71	0	0

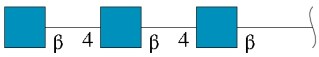
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	948	7570	4803	1269	1467	31	0	0

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

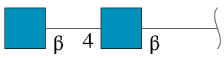
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	324	2575	1619	467	479	10	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	B	3	42	24	3	15	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

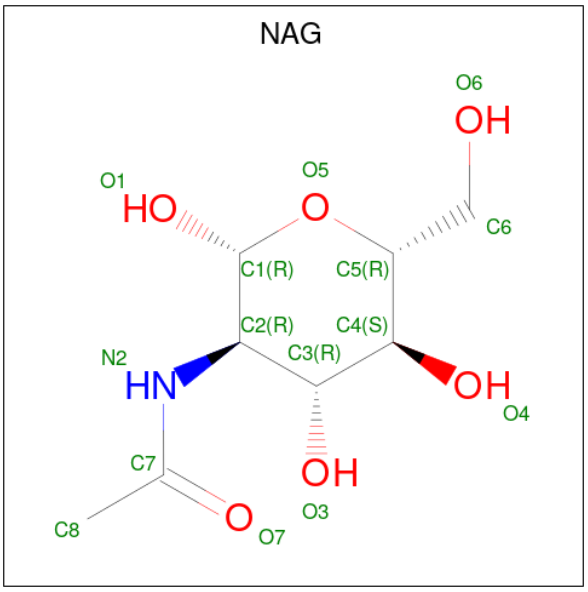
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	D	1	Total	Ca	0
			1	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

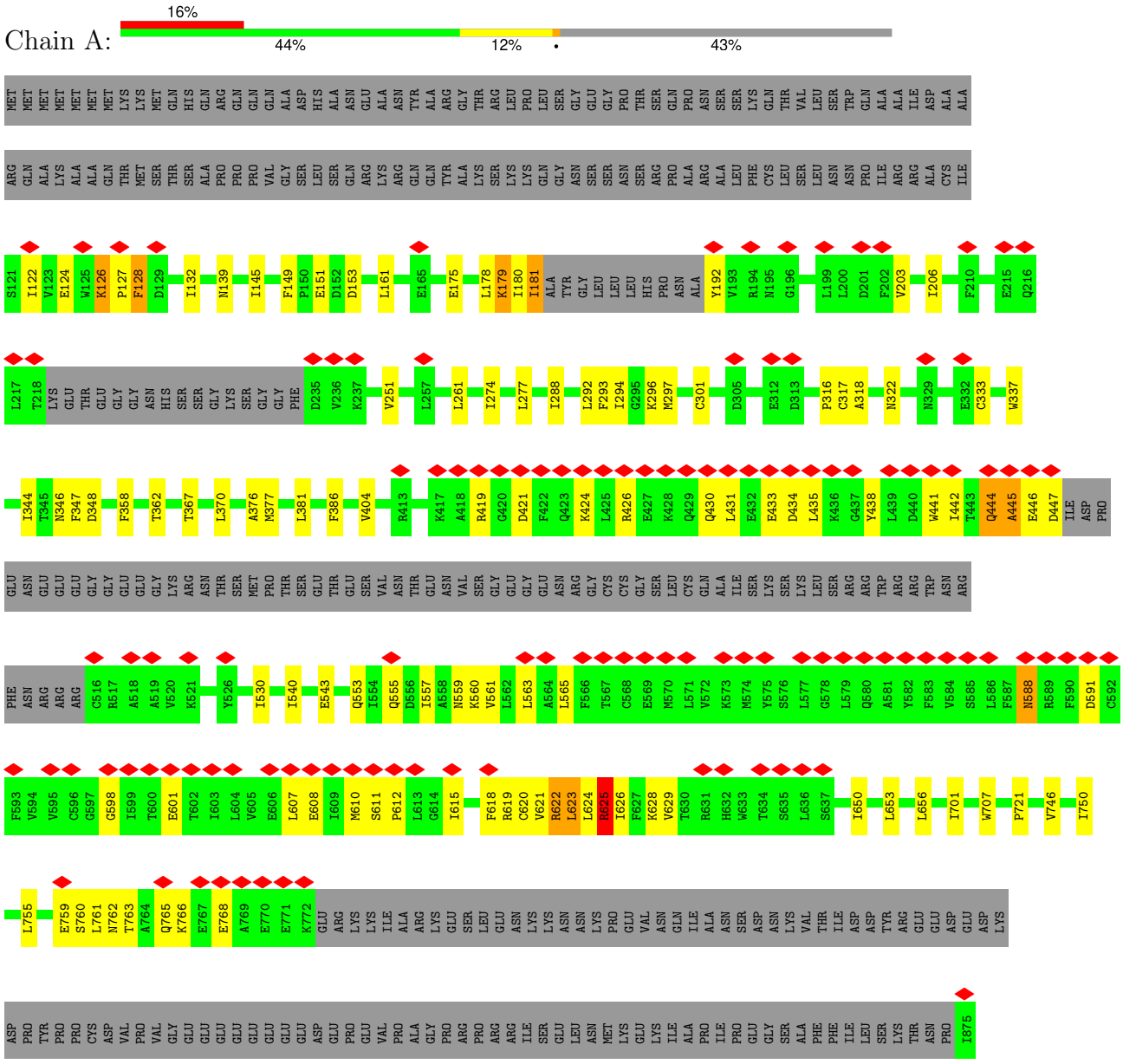


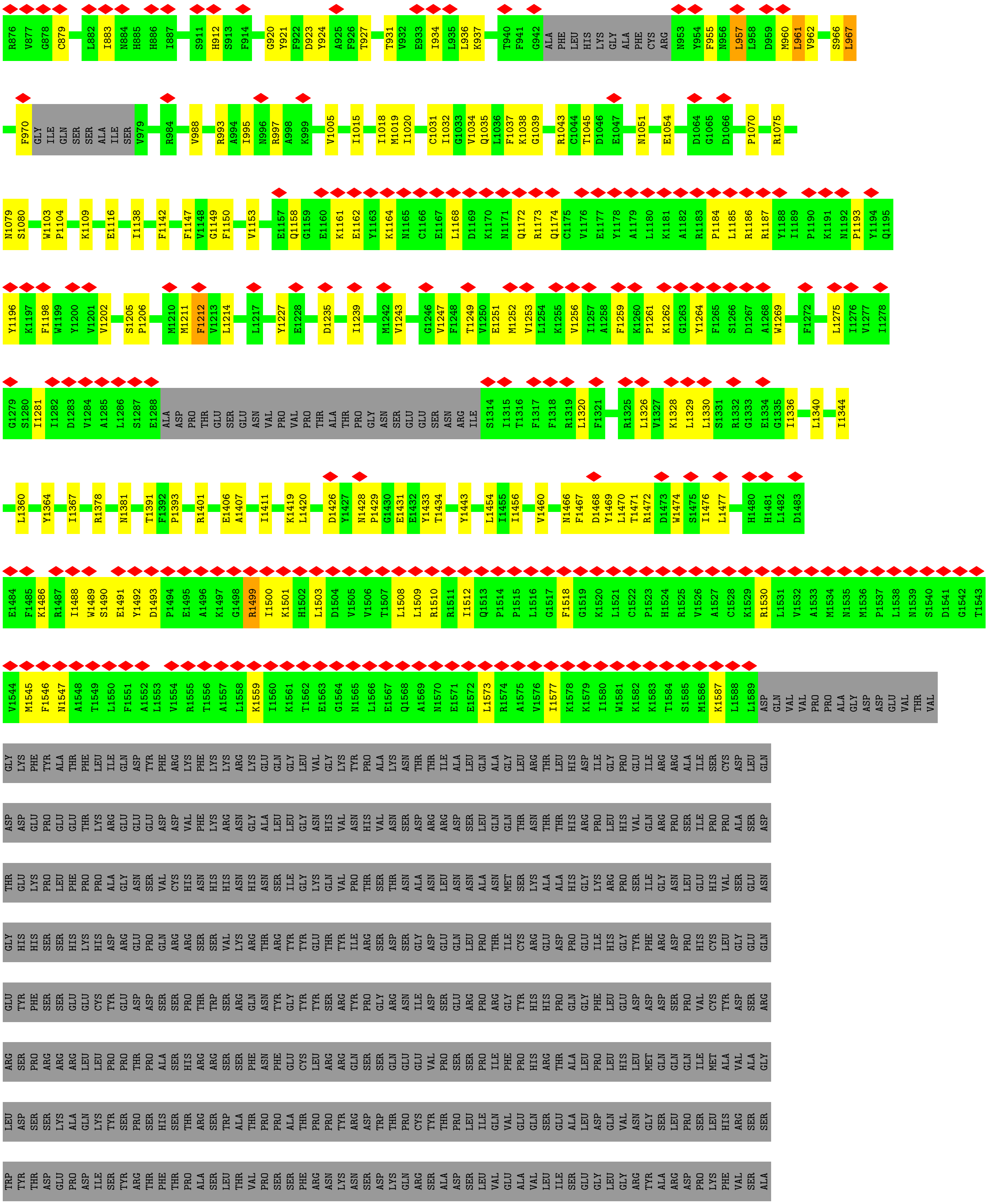
Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	

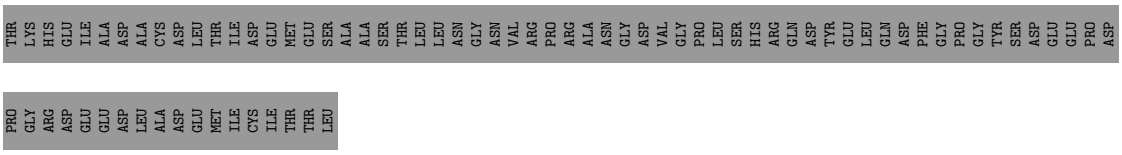
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1D

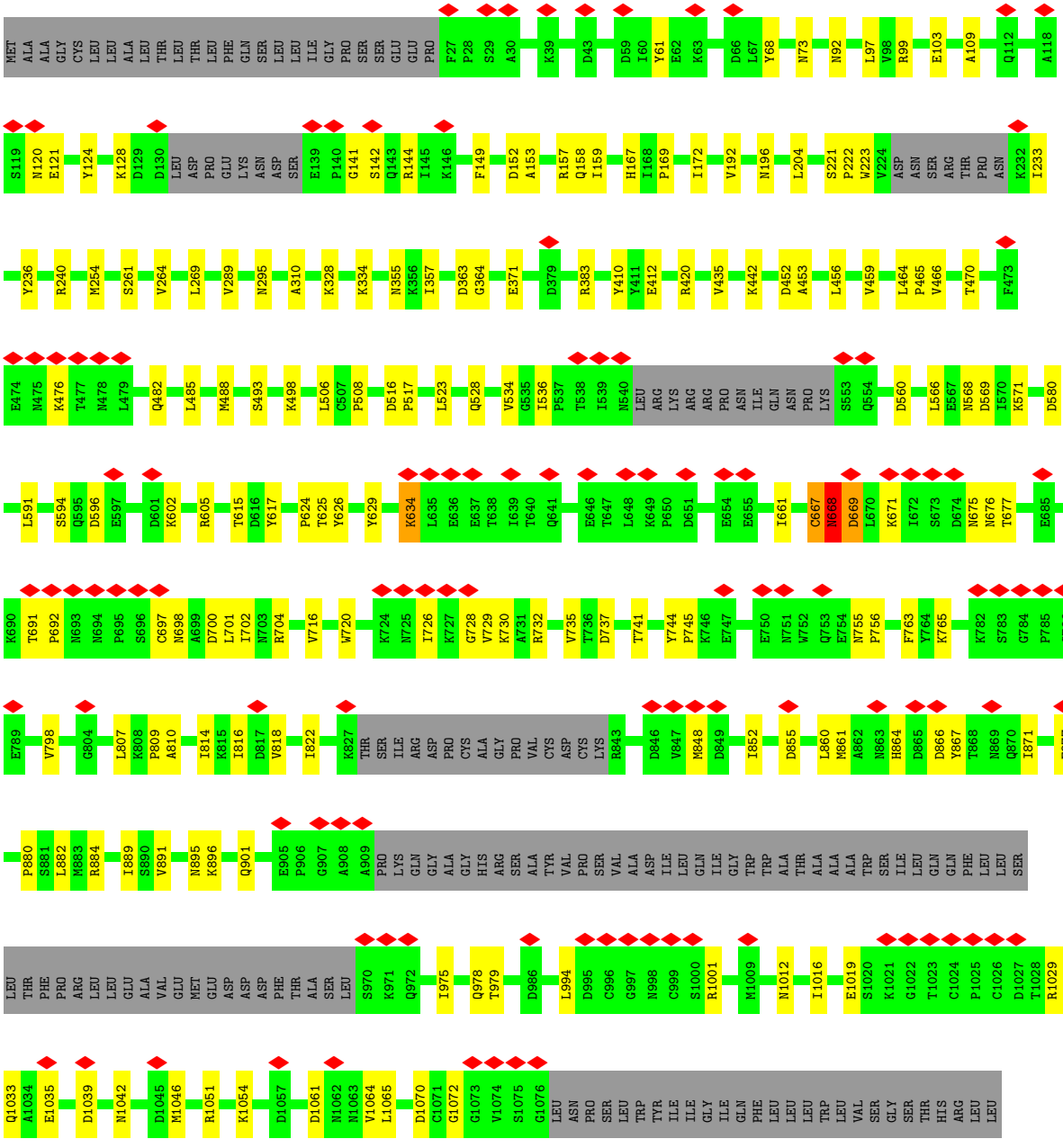



R876 V877 G878 C879 L882 I883 N884 H885 H886 I887 S911 H912 S913 F914 G920 Y921 F922 D923 Y924 A925 F926 T927 T931 V932 E933 I934 L935 L936 K937 T940 F941 G942 ALA PHE LEU HIS LYS GLY ALA PHE CYS ARG N953 Y954 F955 N956 L957 L958 D959 M960 L961 V962 S966 L967
F970 GLY ILE GLN SER SER ALA ILE SER V979 R984 V988 R993 A994 I995 N996 R997 A998 K999 V1005 I1015 I1018 M1019 I1020 C1031 I1032 G1033 V1034 Q1035 L1036 F1037 K1038 G1039 R1043 C1044 T1045 D1046 E1047 N1051 E1054 D1064 G1065 D1066 P1070 R1075
N1079 S1080 W1103 P1104 K1109 E116 I1138 F1142 F1147 V1148 G1149 F1150 V1153 E1157 Q1158 G1159 E1160 K1161 E1162 Y1163 K1164 N1165 C1166 E1167 L1168 D1169 K1170 N1171 Q1172 R1173 Q1174 C1175 V1176 E1177 Y1178 A1179 L1180 K1181 A1182 R1183 P1184 L1185 R1186 R1187 Y1188 I1189 P1190 K1191 N1192 P1193 Y1194 Q1195
Y1196 K1197 F1198 W1199 Y1200 V1201 V1202 S1205 P1206 M1210 M1211 F1212 V1213 L1214 L1217 Y1227 E1228 D1235 I1239 M1242 V1243 G1246 V1247 F1248 T1249 V1250 E1251 M1252 V1253 L1254 K1255 V1256 I1257 A1258 F1259 K1260 P1261 K1262 G1263 Y1264 F1265 S1266 D1267 A1268 W1269 F1272 L1275 I1276 V1277 I1278
G1279 S1280 I1281 I1282 D1283 V1284 A1285 L1286 S1287 E1288 ALA ASP PRO THR GLU SER GLU ASN VAL PRO VAL PRO THR ALA THR PRO GLY ASN SER GLU GLU SER ASN ARG ILE S1314 I1315 T1316 F1317 F1318 R1319 L1320 F1321 R1325 L1326 V1327 K1328 L1329 L1330 S1331 R1332 G1333 E1334 G1335 I1336 L1340 I1344
L1360 Y1364 I1367 R1378 N1381 T1391 F1392 P1393 R1401 E1406 A1407 I1411 K1419 L1420 D1426 Y1427 N1428 P1429 G1430 E1431 E1432 Y1433 T1434 Y1443 L1454 I1455 I1456 V1460 N1466 F1467 D1468 Y1469 L1470 T1471 R1472 D1473 W1474 S1475 I1476 L1477 H1480 H1481 L1482 D1483
E1484 F1485 K1486 R1487 I1488 W1489 S1490 E1491 Y1492 D1493 P1494 E1495 A1496 K1497 G1498 R1499 I1500 K1501 H1502 L1503 D1504 V1505 V1506 T1507 L1508 L1509 R1510 R1511 I1512 Q1513 P1514 P1515 L1516 G1517 F1518 G1519 K1520 L1521 C1522 P1523 H1524 R1525 V1526 A1527 C1528 K1529 R1530 L1531 V1532 A1533 M1534 N1535 M1536 P1537 L1538 N1539 S1540 D1541 G1542 T1543
V1544 M1545 F1546 N1547 A1548 T1549 L1550 F1551 A1552 L1553 V1554 R1555 T1556 A1557 L1558 K1559 I1560 K1561 T1562 E1563 G1564 N1565 L1566 E1567 Q1568 A1569 N1570 E1571 E1572 L1573 R1574 A1575 V1576 I1577 K1578 K1579 I1580 W1581 K1582 K1583 T1584 S1585 M1586 K1587 L1588 L1589 ASP GLN VAL VAL PRO PRO ALA GLY ASP ASP GLU VAL THR VAL
GLY LYS PHE TYR ALA THR PHE LEU ILE GLN ASP TYR PHE ARG LYS PHE LYS LYS ARG LYS GLU GLN GLY LEU VAL GLY LYS TYR PRO ALA LYS ASN THR THR ILE ALA LEU GLN ALA GLY LEU ARG THR LEU HIS ASP ILE GLY PRO GLU ILE ARG ARG ALA ILE SER CYS ASP LEU GLN
ASP ASP GLU PRO GLU GLU THR LYS ARG GLU GLU GLU ASP ASP VAL PHE LYS ARG ASN GLY ALA LEU LEU GLY ASN HIS VAL ASN HIS VAL ASN SER ASP ARG ARG ASP SER LEU GLN GLN THR ASN THR THR HIS ARG PRO LEU HIS VAL GLN ARG PRO SER ILE PRO PRO ALA SER ASP
THR GLU LYS PRO LEU PHE PRO PRO ALA GLY ASN SER VAL CYS HIS ASN HIS HIS ASN HIS ASN SER ILE GLY LYS GLN VAL PRO THR SER THR ASN ALA ASN LEU ASN ASN ALA ASN MET SER LYS ALA ALA HIS GLY LYS ARG PRO SER ILE GLY ASN LEU GLU HIS VAL SER GLU ASN
GLY HIS HIS SER SER HIS LYS HIS ASP ARG GLU PRO GLN ARG ARG SER SER VAL LYS ARG THR ARG TYR TYR GLU THR TYR ILE ARG SER ASP SER GLY ASP GLU GLN LEU PRO THR ILE CYS ARG GLU ASP PRO GLU ILE HIS GLY TYR PHE ARG ASP PRO HIS CYS LEU GLY GLY GLN
GLU TYR PHE SER SER GLU GLU CYS TYR GLU ASP ASP SER SER PRO THR TRP SER ARG GLN ASN TYR GLY TYR TYR SER ARG TYR PRO GLY ARG ASN ILE ASP SER GLU ARG PRO ARG GLY TYR HIS HIS PRO GLN GLY PHE LEU GLU ASP ASP ASP SER PRO VAL CYS TYR ASP SER ARG
ARG SER PRO ARG ARG ARG LEU LEU PRO PRO THR PRO ALA SER HIS ARG ARG SER SER PHE ASN PHE GLU CYS LEU ARG ARG GLN SER SER GLN GLU GLU VAL PRO SER SER PRO ILE PHE PRO HIS ARG THR ALA LEU PRO LEU HIS LEU MET GLN GLN GLN ILE MET ALA VAL ALA GLY
LEU ASP SER SER LYS ALA GLN LYS TYR SER PRO SER HIS SER THR ARG SER TRP ALA THR PRO PRO ALA THR PRO PRO TYR ARG ASP TRP THR PRO CYS TYR THR PRO LEU ILE GLN VAL GLU GLN SER GLU ALA LEU ASP GLN VAL ASN GLY SER LEU PRO SER LEU HIS ARG SER SER
TRP TYR THR ASP GLU PRO ASP ILE SER TYR ARG THR PHE THR PRO ALA SER LEU THR VAL PRO SER SER PHE ARG ASN LYS ASN SER ASP LYS GLN ARG SER ALA ASP SER LEU VAL GLU ALA VAL LEU ILE SER GLU GLY LEU GLY ARG TYR ALA ARG ASP PRO LYS PHE VAL SER ALA



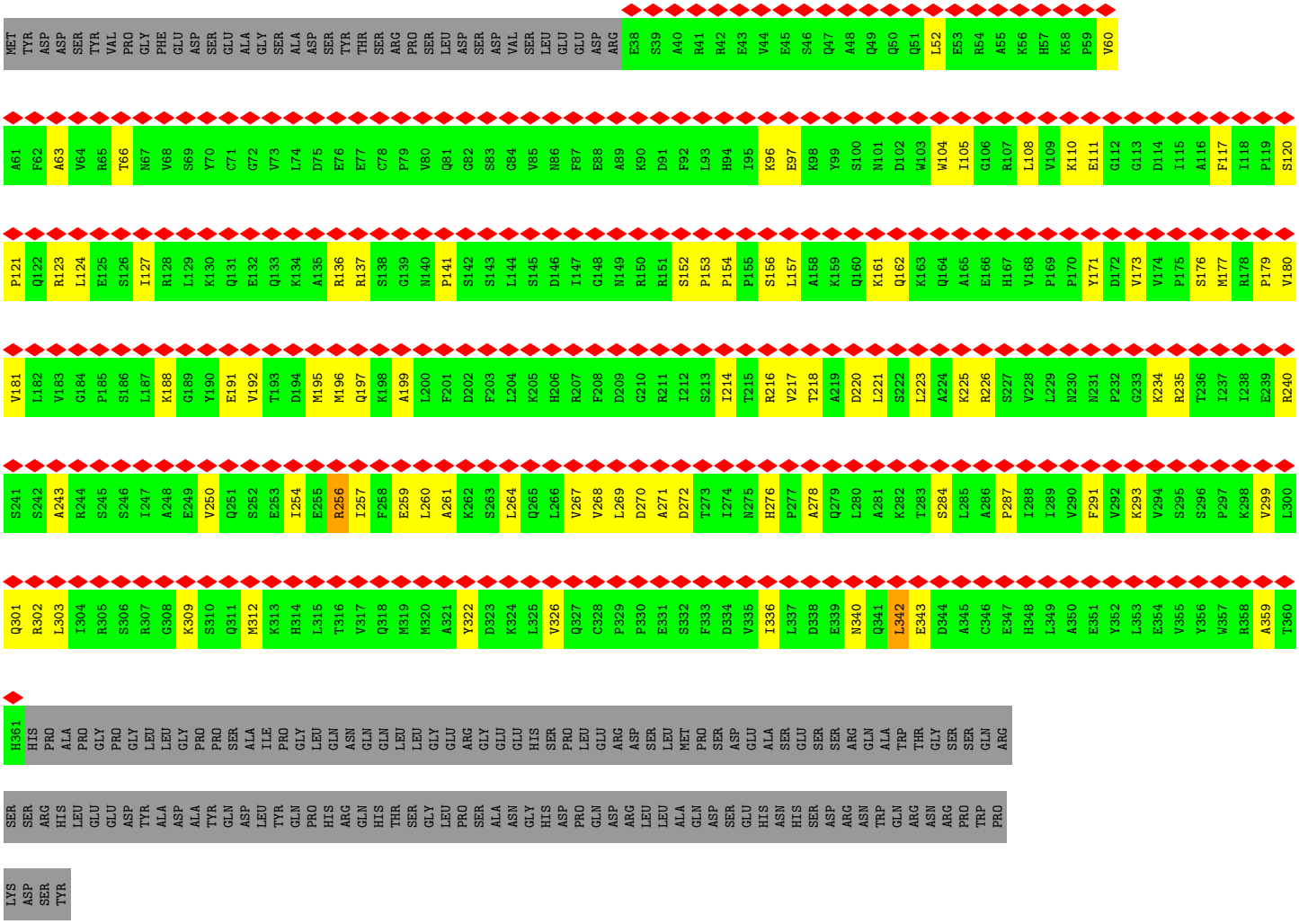
• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:



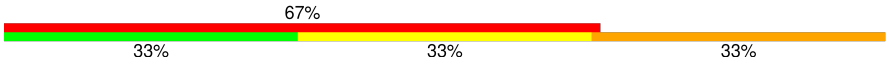
• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

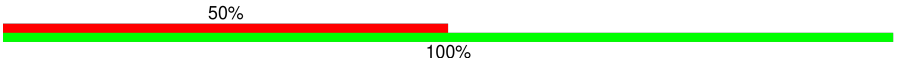


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.097	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/10127	0.47	0/13716
2	D	0.25	0/7728	0.47	0/10477
3	C	0.25	0/2624	0.52	0/3544
All	All	0.25	0/20479	0.48	0/27737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9900	0	10071	232	0
2	D	7570	0	7370	102	0
3	C	2575	0	2619	87	0
4	B	42	0	37	2	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	2	0
6	F	56	0	49	2	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	28	0	26	1	0
All	All	20257	0	20247	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 384 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:TYR:CE1	3:C:340:ASN:HA	1.60	1.36
1:A:442:ILE:HD12	3:C:196:MET:SD	1.77	1.24
1:A:434:ASP:OD1	3:C:340:ASN:ND2	1.74	1.19
1:A:431:LEU:HD11	3:C:299:VAL:HG23	1.27	1.17
1:A:442:ILE:CG1	3:C:196:MET:HG3	1.77	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1214/2161 (56%)	1150 (95%)	60 (5%)	4 (0%)	37 66
2	D	936/1103 (85%)	886 (95%)	49 (5%)	1 (0%)	48 76
3	C	322/484 (66%)	308 (96%)	14 (4%)	0	100 100
All	All	2472/3748 (66%)	2344 (95%)	123 (5%)	5 (0%)	45 71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	668	ASN
1	A	625	ARG

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Mol	Chain	Res	Type
1	A	126	LYS
1	A	444	GLN
1	A	445	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1086/1902 (57%)	1055 (97%)	31 (3%)	37	63
2	D	837/971 (86%)	830 (99%)	7 (1%)	79	87
3	C	287/426 (67%)	285 (99%)	2 (1%)	81	88
All	All	2210/3299 (67%)	2170 (98%)	40 (2%)	54	74

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1212	PHE
2	D	669	ASP
1	A	1214	LEU
2	D	634	LYS
2	D	697	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	559	ASN
2	D	676	ASN
2	D	698	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

13 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1	4,2	14,14,15	0.35	0	17,19,21	0.57	0
4	NAG	B	2	4	14,14,15	0.38	0	17,19,21	1.34	2 (11%)
4	NAG	B	3	4	14,14,15	0.36	0	17,19,21	0.40	0
5	NAG	E	1	5,2	14,14,15	0.31	0	17,19,21	0.57	0
5	NAG	E	2	5	14,14,15	0.46	0	17,19,21	0.81	0
6	NAG	F	1	6,2	14,14,15	0.18	0	17,19,21	0.47	0
6	NAG	F	2	6	14,14,15	0.28	0	17,19,21	0.39	0
6	NAG	F	3	6	14,14,15	0.96	1 (7%)	17,19,21	1.74	3 (17%)
6	NAG	F	4	6	14,14,15	0.52	0	17,19,21	1.34	2 (11%)
5	NAG	G	1	5,2	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	G	2	5	14,14,15	0.34	0	17,19,21	0.51	0
5	NAG	H	1	5,2	14,14,15	0.76	1 (7%)	17,19,21	1.30	1 (5%)
5	NAG	H	2	5	14,14,15	0.23	0	17,19,21	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	4/6/23/26	0/1/1/1
4	NAG	B	3	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	6/6/23/26	0/1/1/1
6	NAG	F	4	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.10	1.48	1.43
5	H	1	NAG	O5-C1	2.05	1.47	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1	NAG	C1-O5-C5	4.93	118.79	112.19
6	F	3	NAG	C2-N2-C7	4.67	129.16	122.90
6	F	3	NAG	C1-O5-C5	4.65	118.42	112.19
4	B	2	NAG	C2-N2-C7	4.57	129.03	122.90
6	F	4	NAG	C2-N2-C7	4.57	129.02	122.90

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C4-C5-C6-O6
6	F	3	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	3	NAG	1	0

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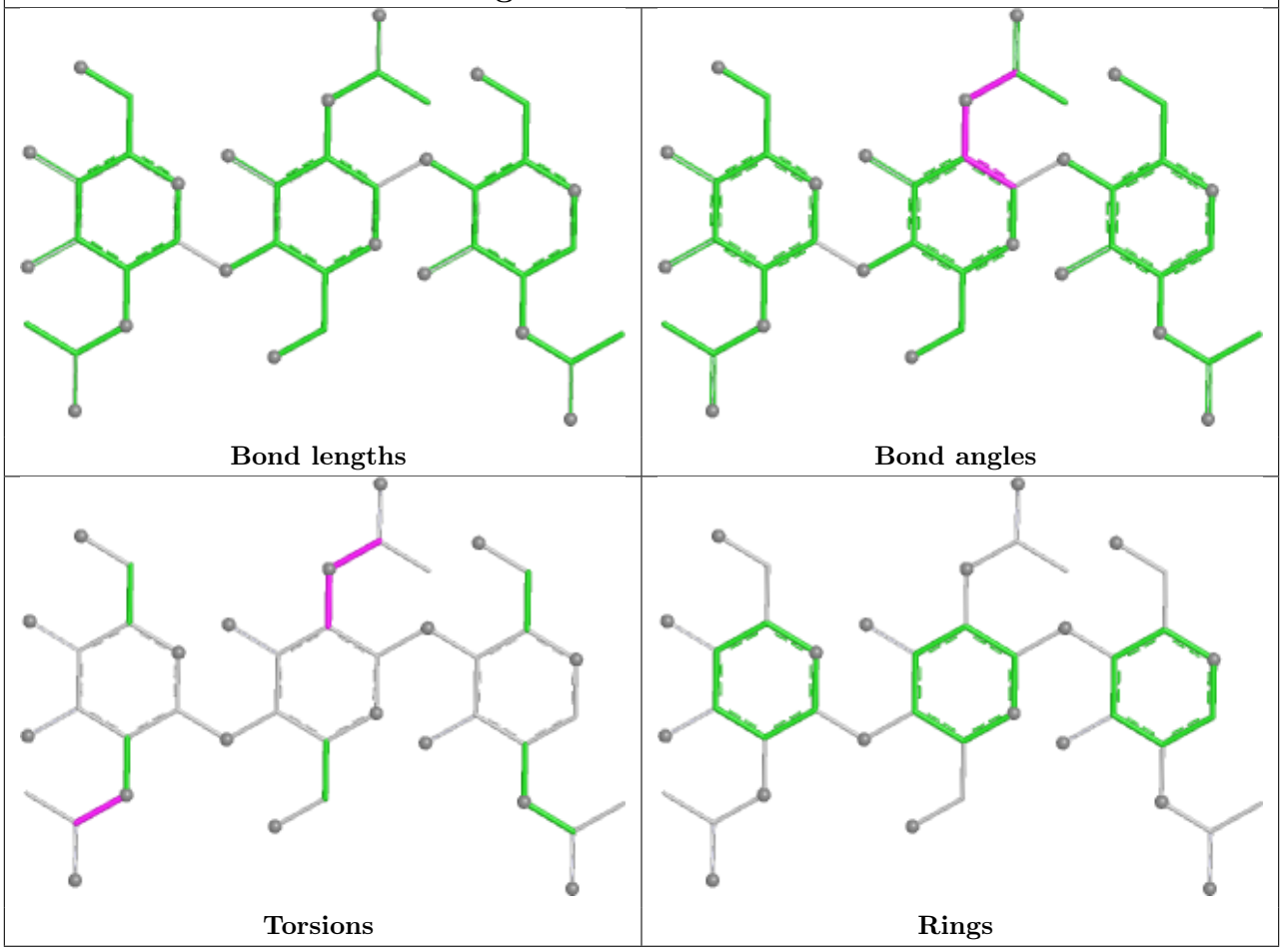
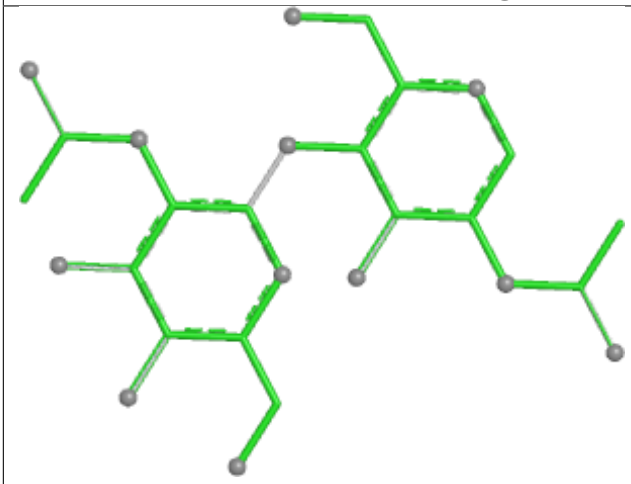
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	2	0
4	B	1	NAG	1	0
6	F	4	NAG	1	0
4	B	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

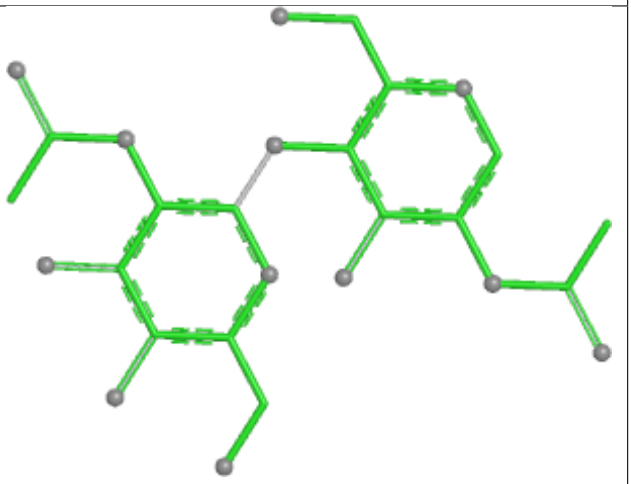
Oligosaccharide Chain B



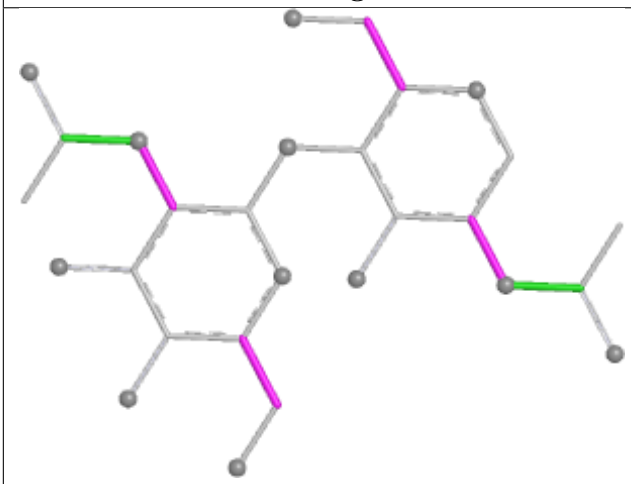
Oligosaccharide Chain E



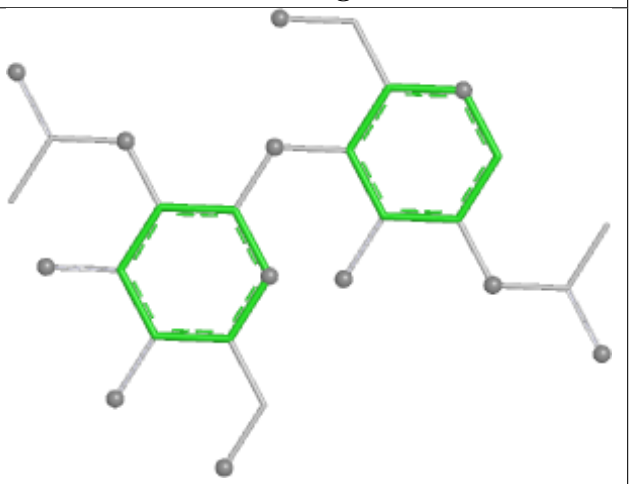
Bond lengths



Bond angles

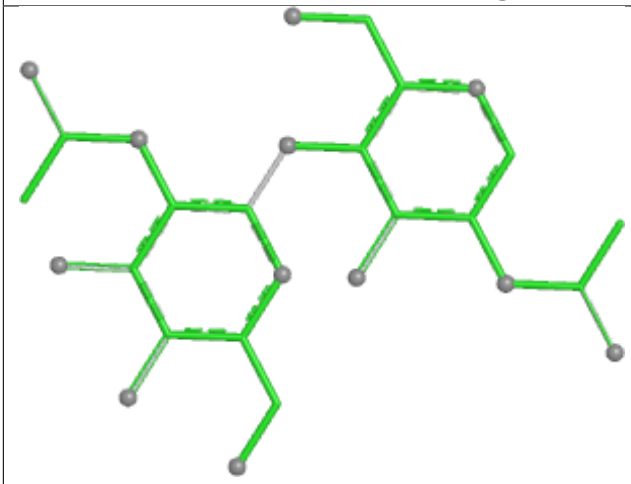


Torsions

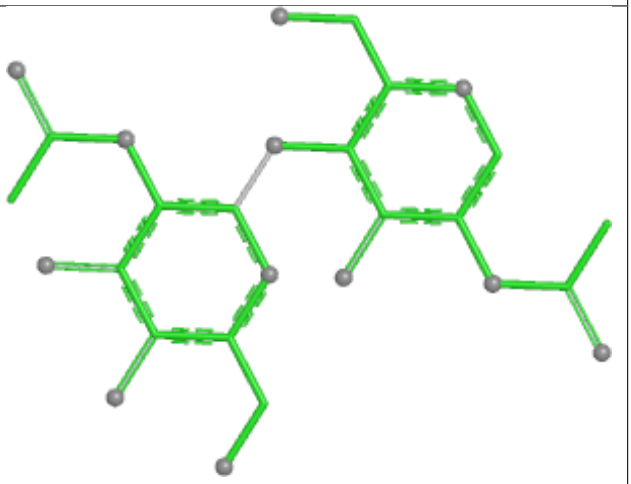


Rings

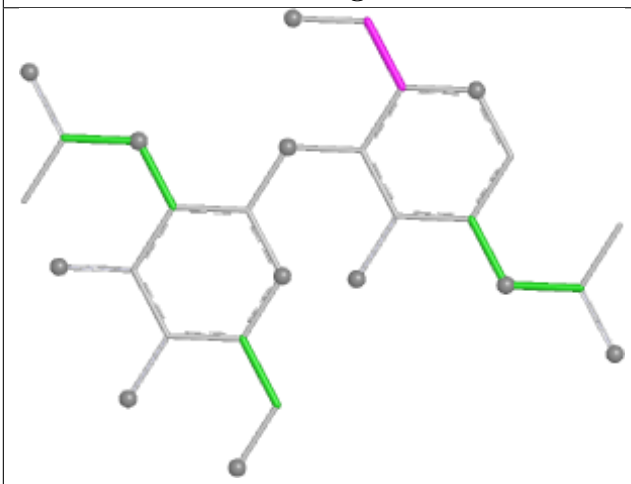
Oligosaccharide Chain G



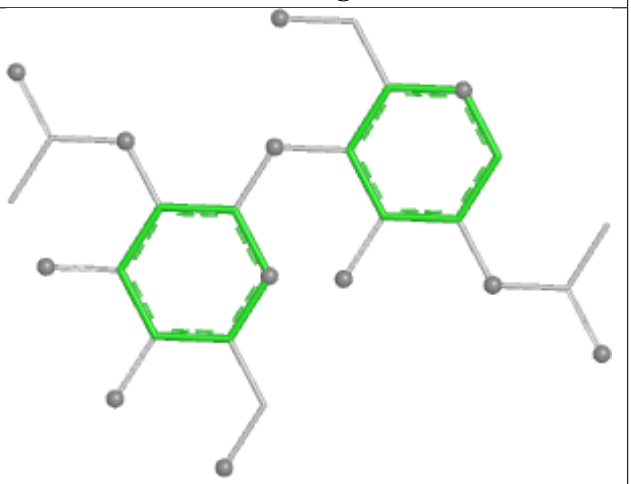
Bond lengths



Bond angles

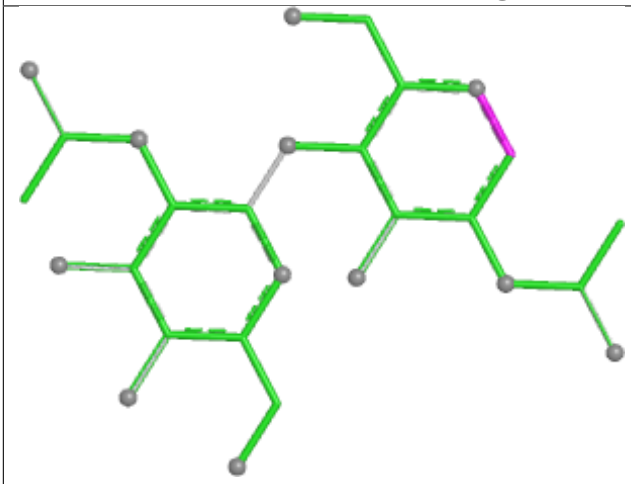


Torsions

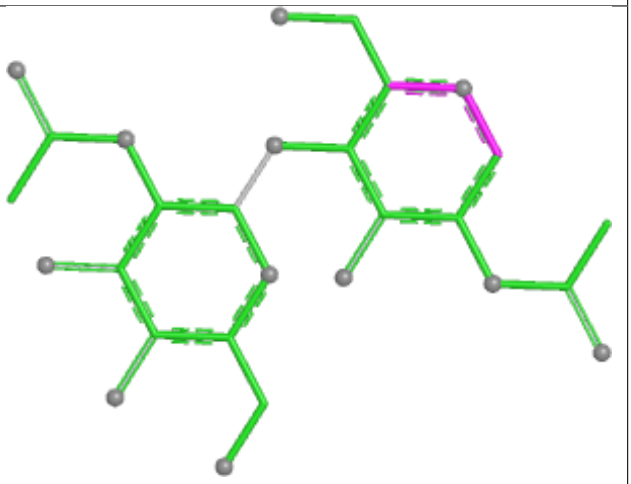


Rings

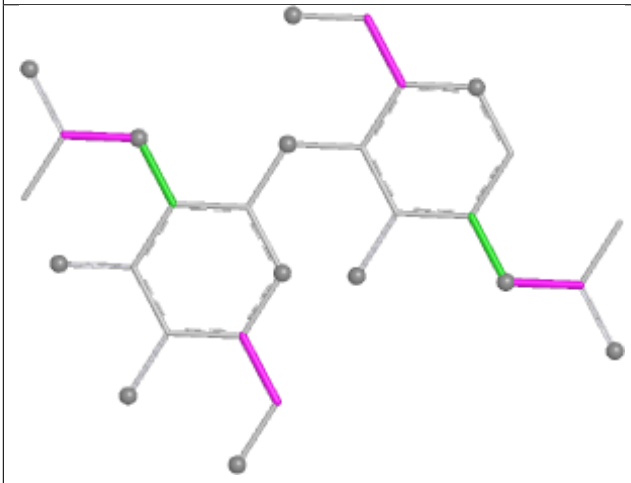
Oligosaccharide Chain H



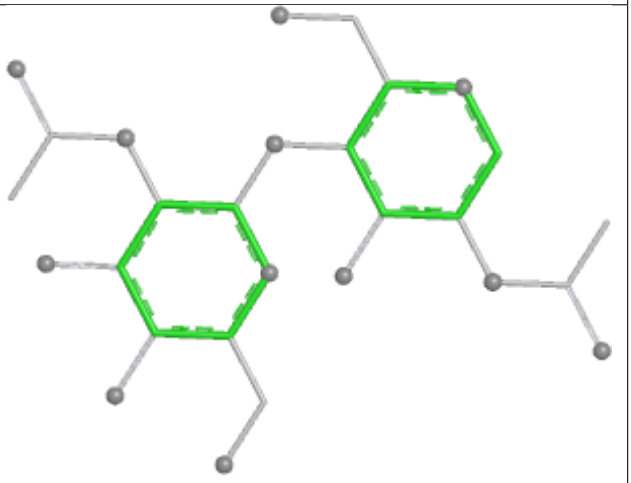
Bond lengths



Bond angles

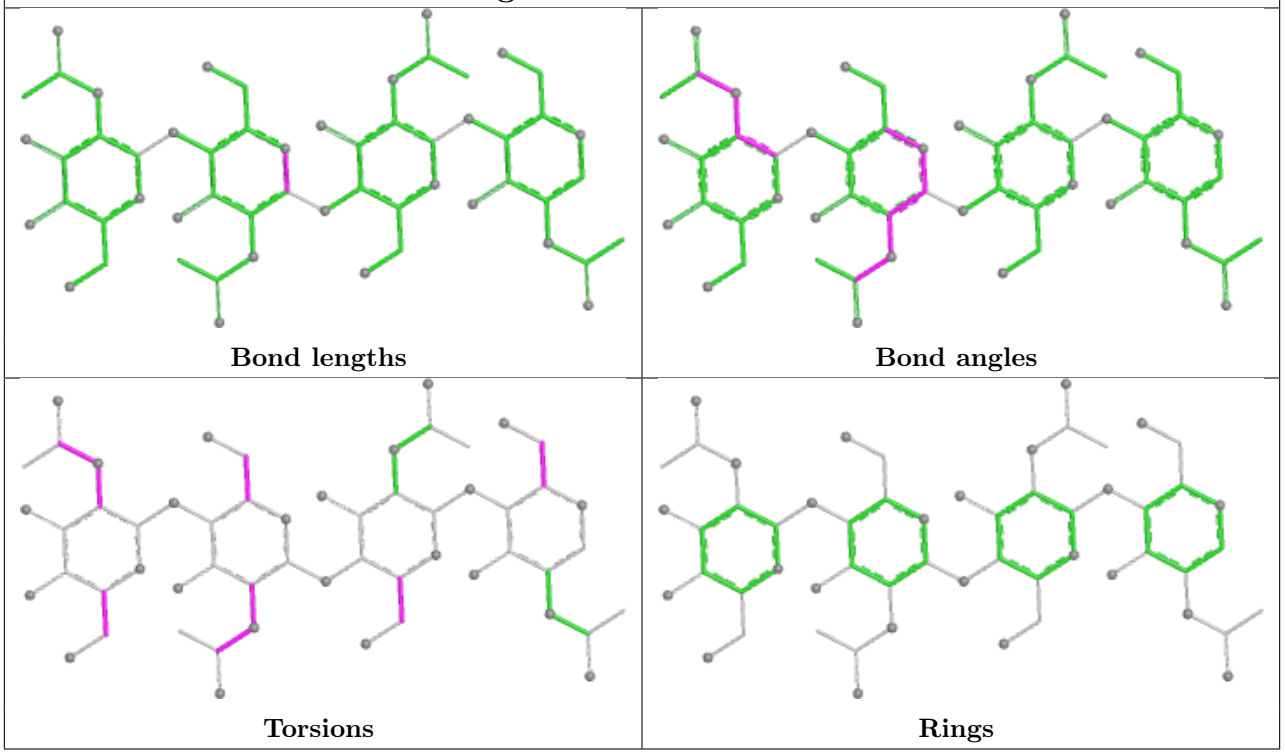


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	D	1202	-	14,14,15	0.22	0	17,19,21	0.43	0
8	NAG	D	1201	2	14,14,15	0.41	0	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	1202	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	1201	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	1201	NAG	O5-C5-C6-O6
8	D	1201	NAG	C4-C5-C6-O6
8	D	1201	NAG	C3-C2-N2-C7
8	D	1201	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1201	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

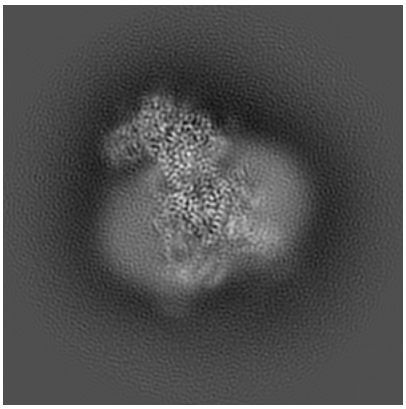
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27908. These allow visual inspection of the internal detail of the map and identification of artifacts.

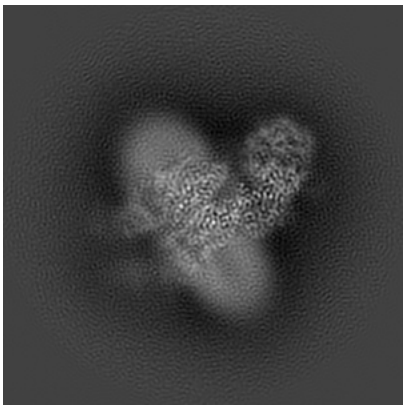
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

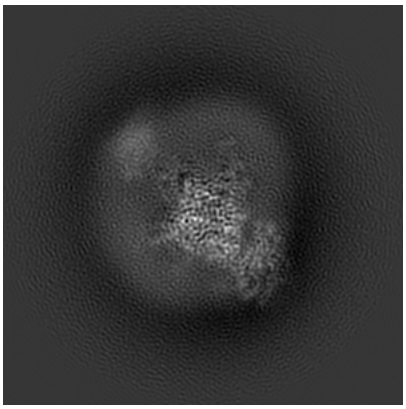
6.1.1 Primary map



X

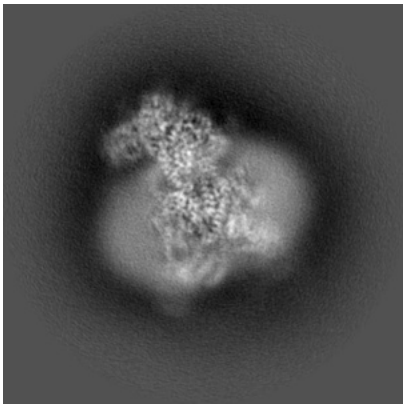


Y

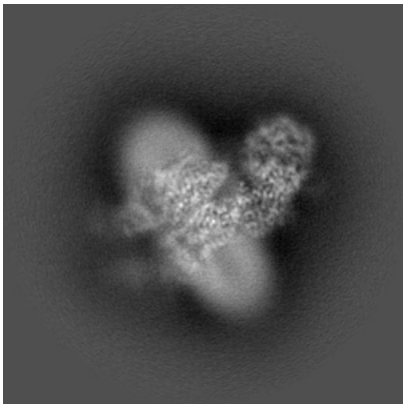


Z

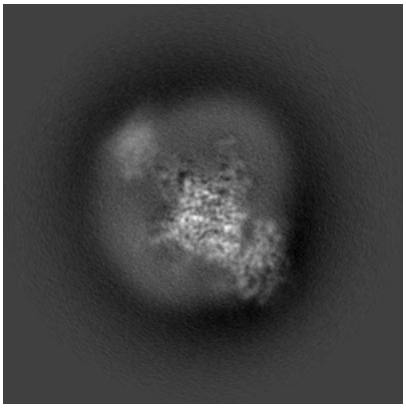
6.1.2 Raw map



X



Y

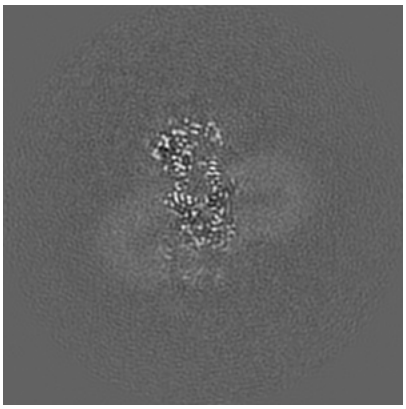


Z

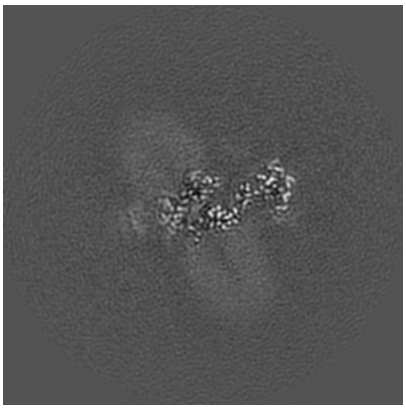
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

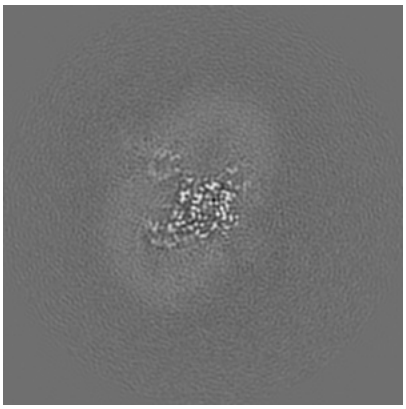
6.2.1 Primary map



X Index: 140

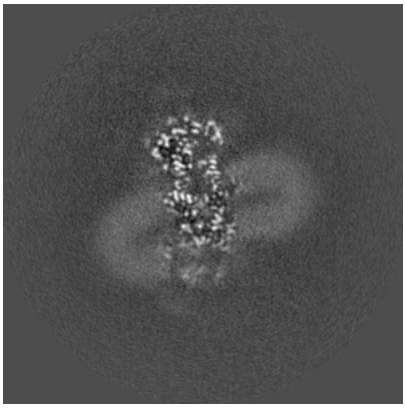


Y Index: 140

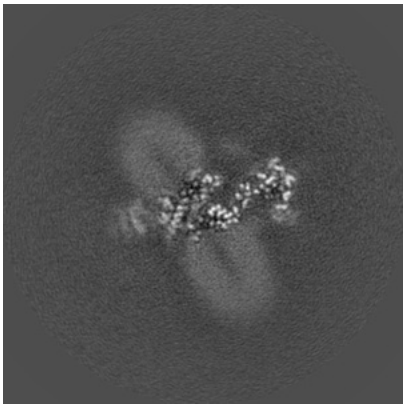


Z Index: 140

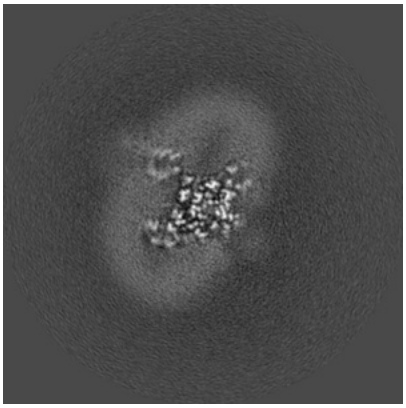
6.2.2 Raw map



X Index: 140



Y Index: 140

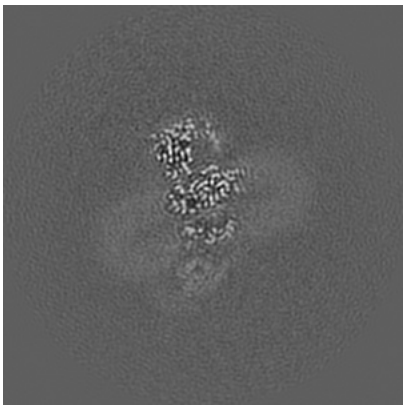


Z Index: 140

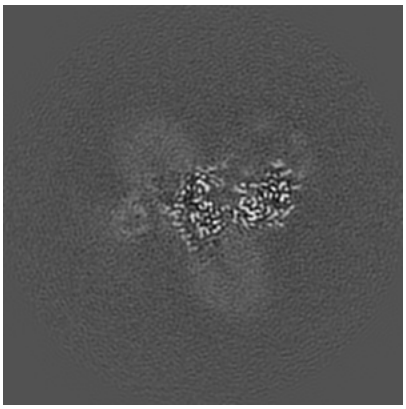
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

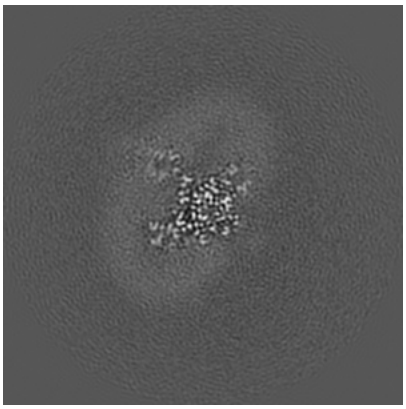
6.3.1 Primary map



X Index: 135

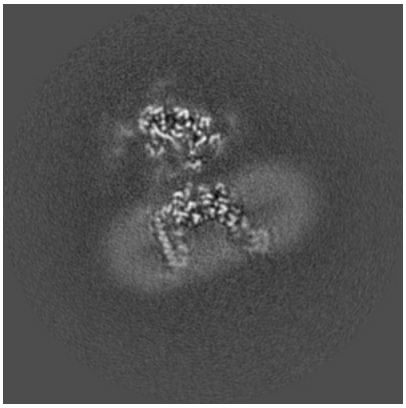


Y Index: 130

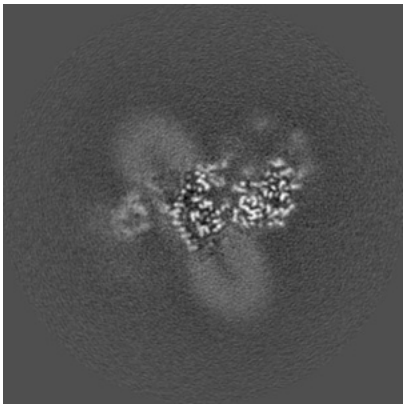


Z Index: 141

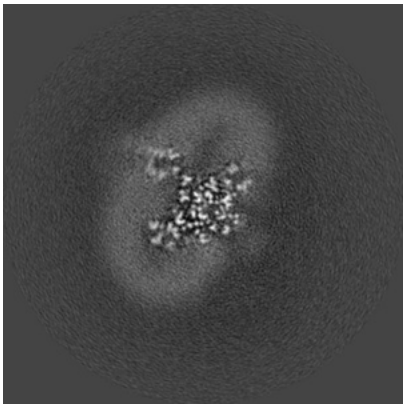
6.3.2 Raw map



X Index: 155



Y Index: 130

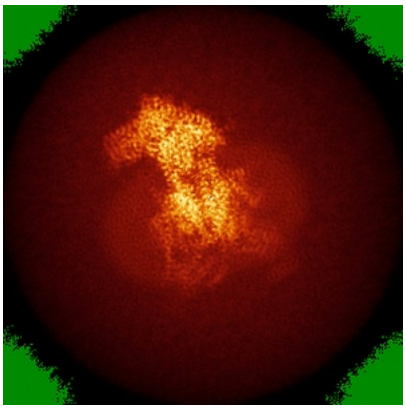


Z Index: 141

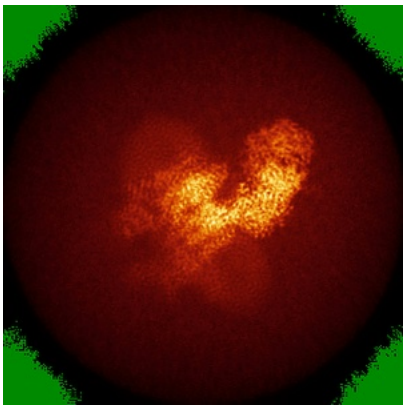
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

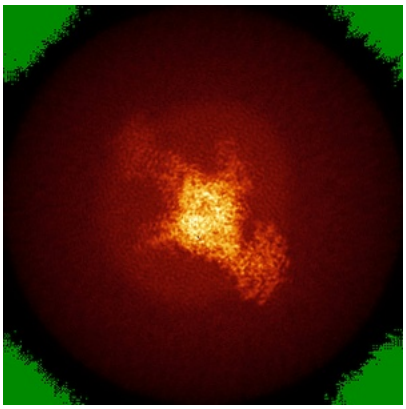
6.4.1 Primary map



X

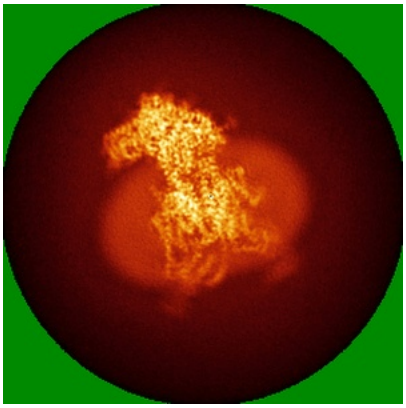


Y

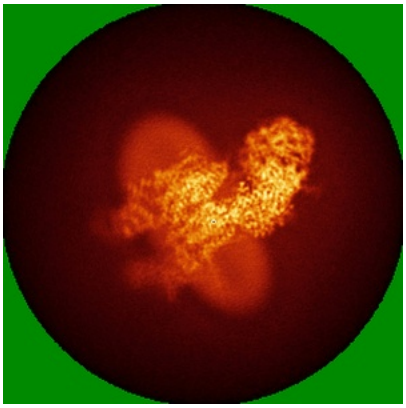


Z

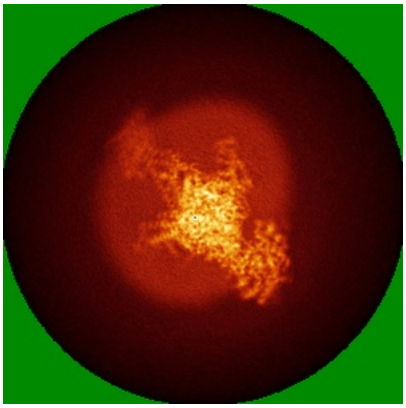
6.4.2 Raw map



X



Y

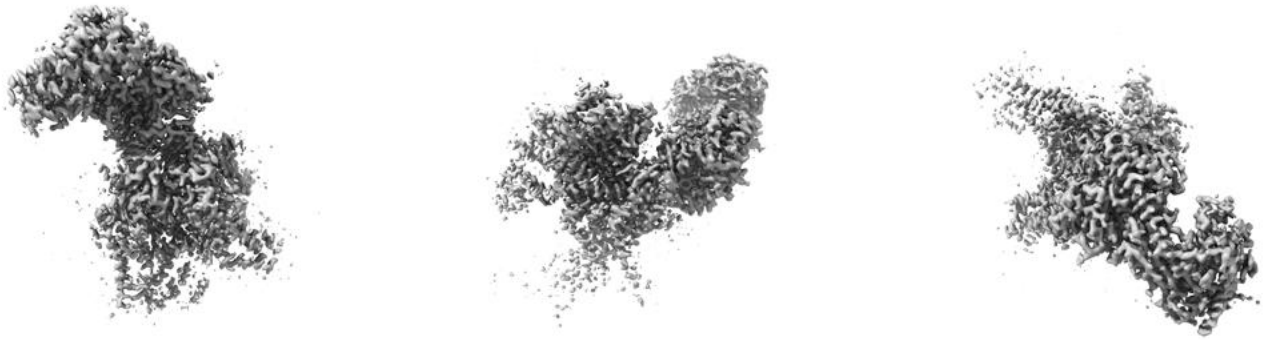


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

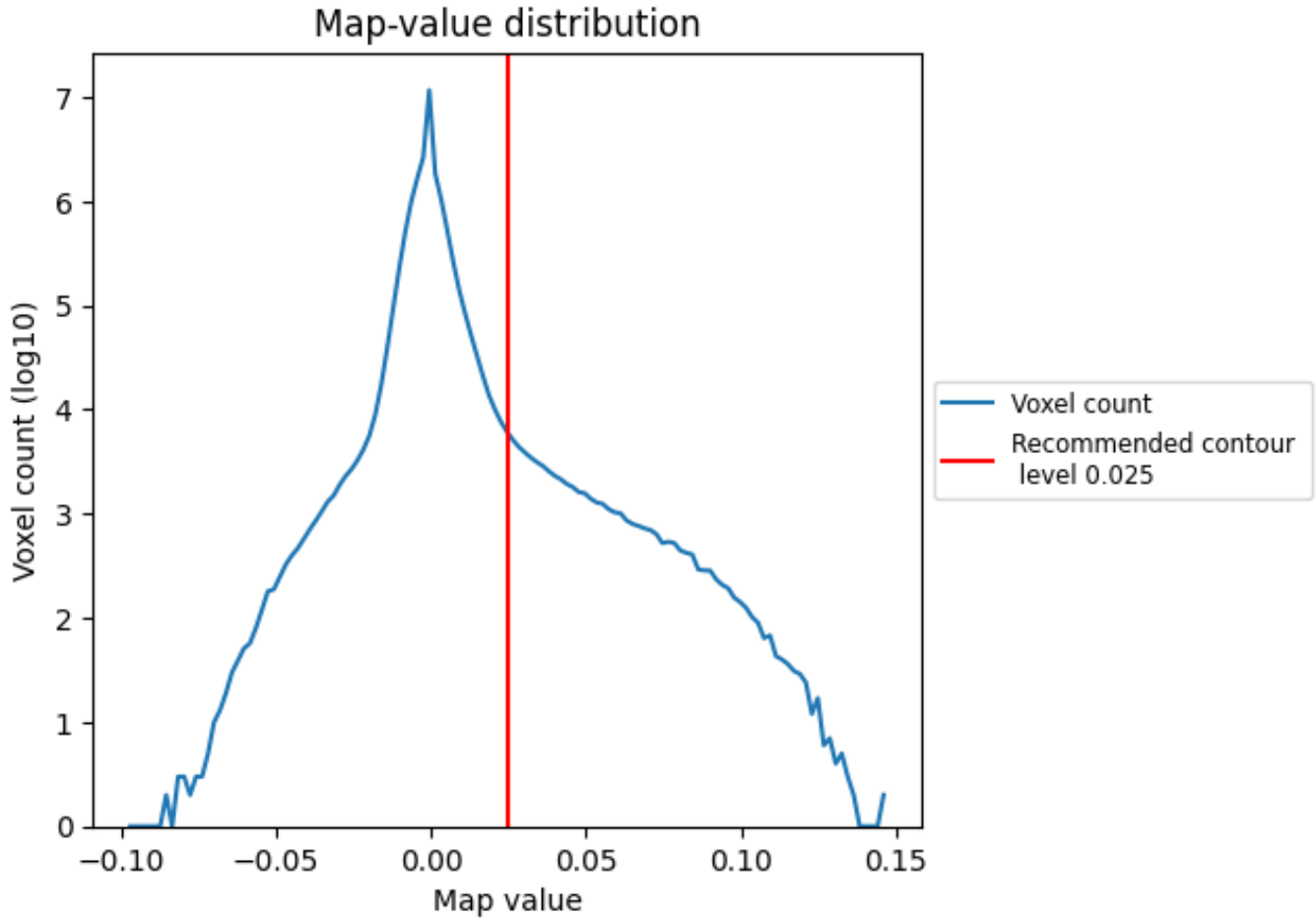
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

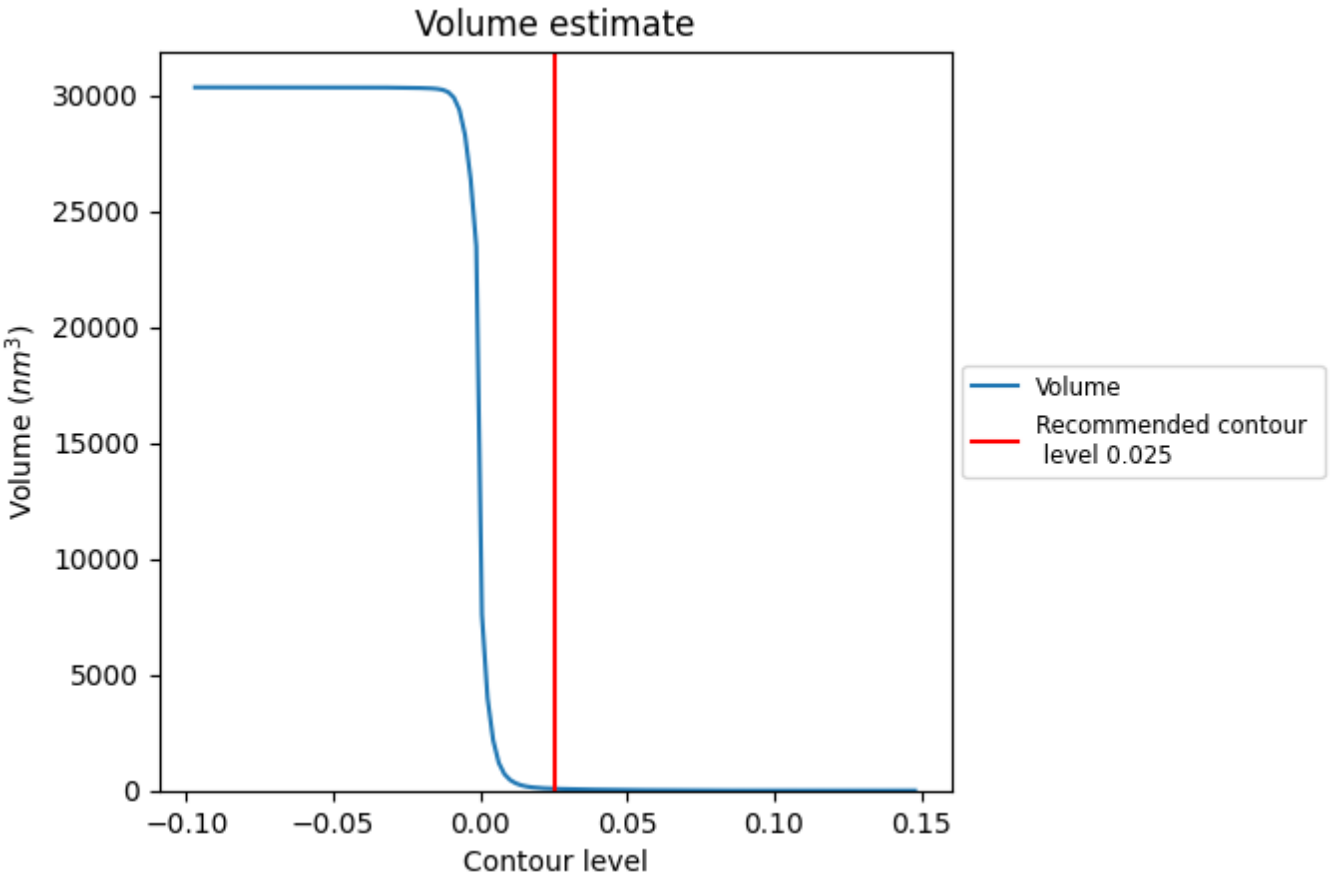
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

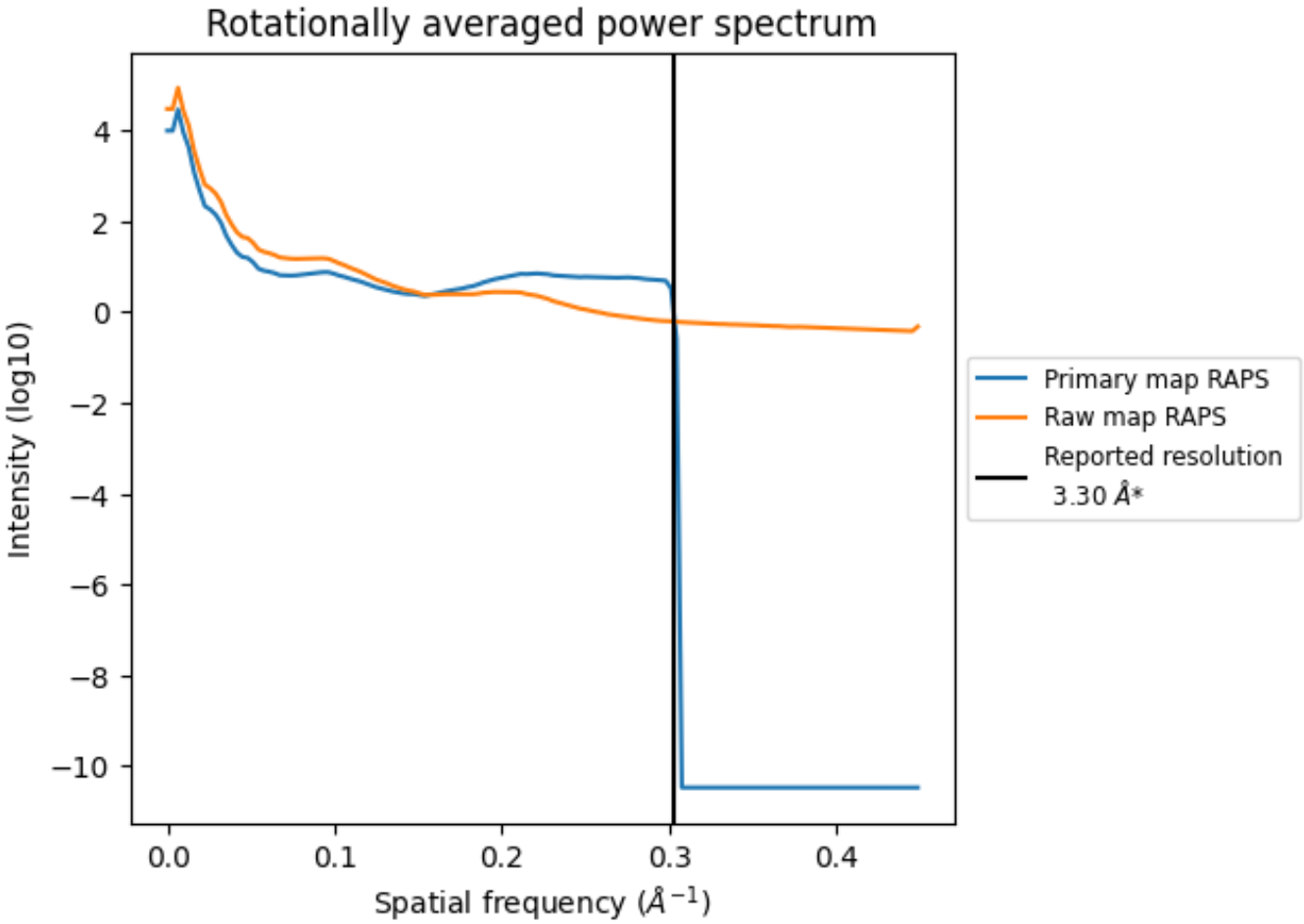
7.2 Volume estimate (i)



The volume at the recommended contour level is 80 nm^3; this corresponds to an approximate mass of 73 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

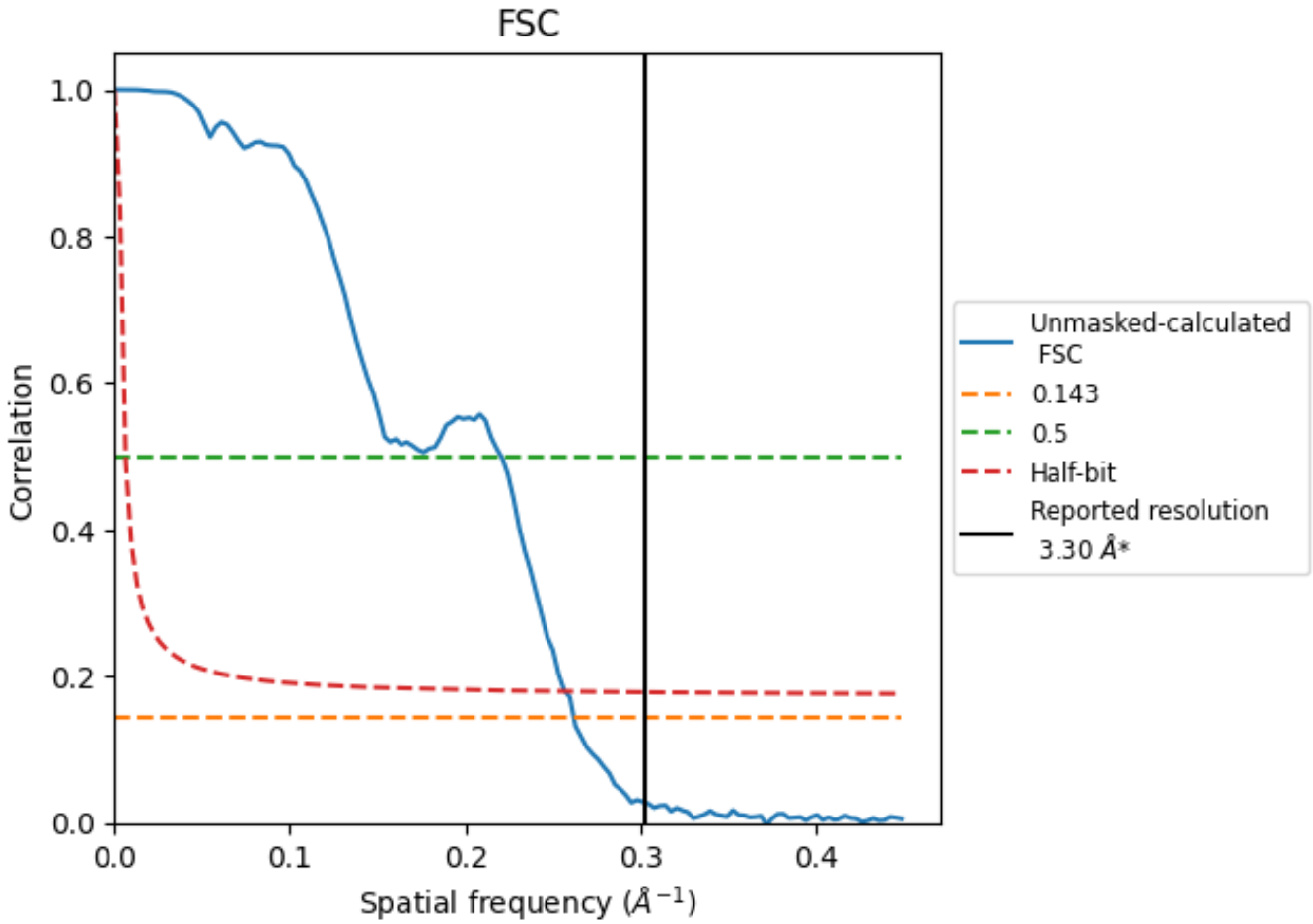


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

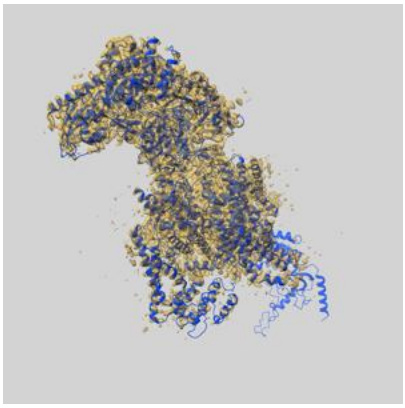
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.54	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.3 by more than 10 %

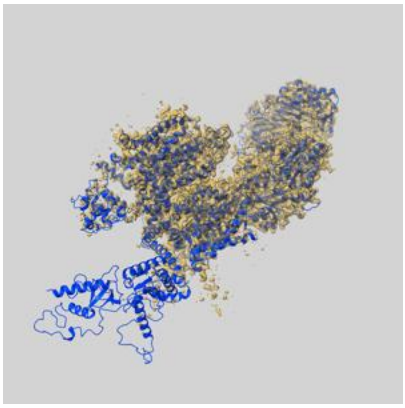
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27908 and PDB model 8E5A. Per-residue inclusion information can be found in section 3 on page 6.

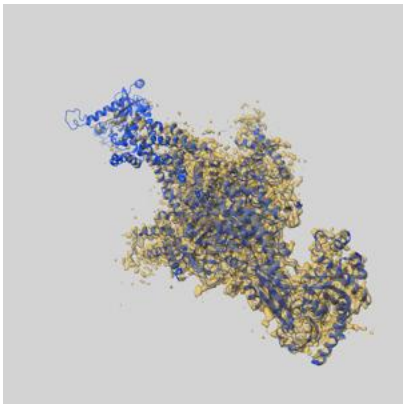
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

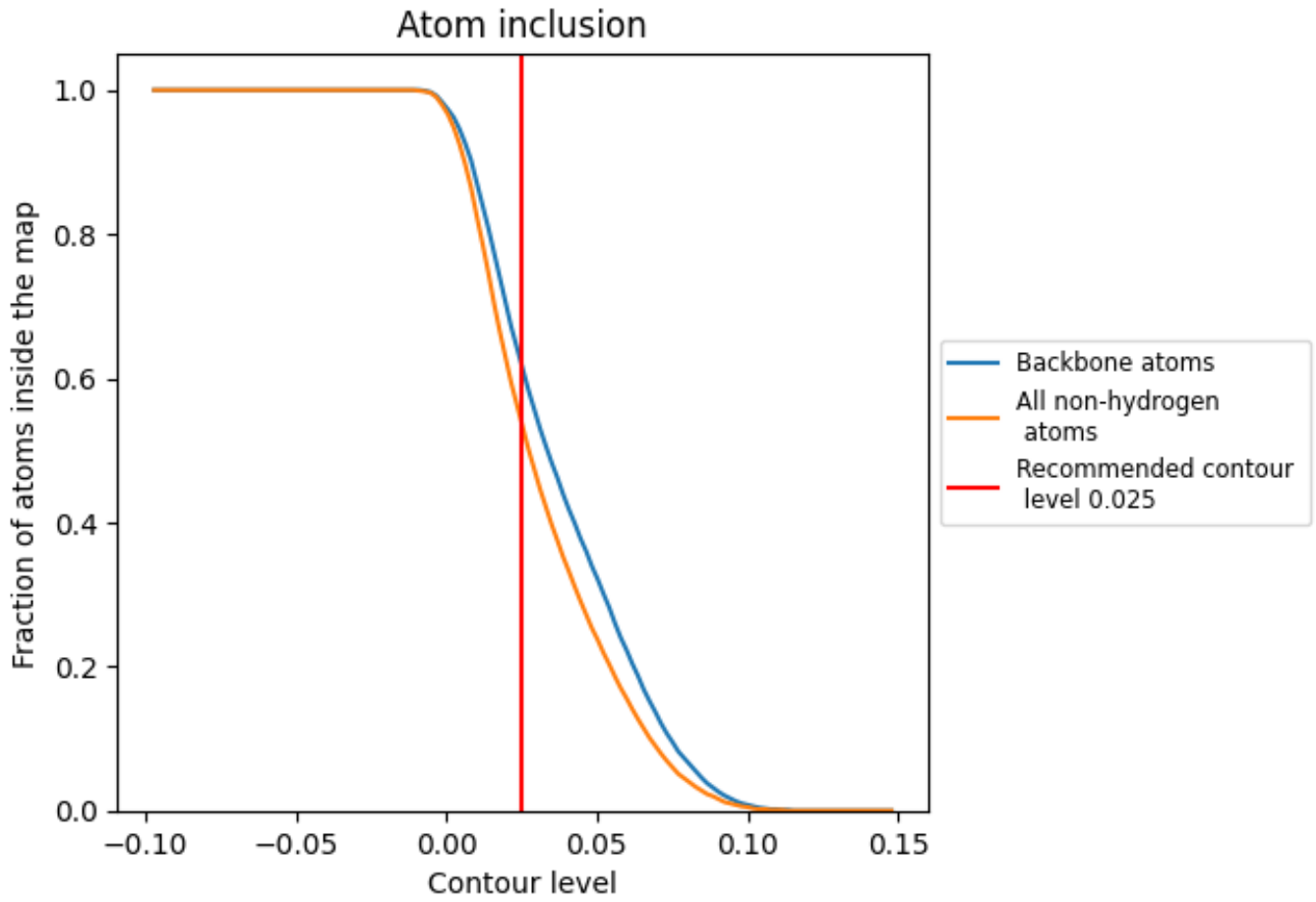
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.4230
A	0.5570	0.4490
B	0.2860	0.3110
C	0.0090	0.0670
D	0.6950	0.5090
E	0.1790	0.3010
F	0.5000	0.4190
G	0.2860	0.4120
H	0.3930	0.3500